

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> e paspalinine

|     |       |                |
|-----|-------|----------------|
| E1  | 2     | PASPALINIC/BI  |
| E2  | 1     | PASPALININ/BI  |
| E3  | 6 --> | PASPALININE/BI |
| E4  | 3     | PASPALITREM/BI |
| E5  | 4     | PASPALOIDES/BI |
| E6  | 35    | PASPALUM/BI    |
| E7  | 1     | PASPAT/BI      |
| E8  | 1     | PASPER/BI      |
| E9  | 5     | PASPER2/BI     |
| E10 | 1     | PASPERTIN/BI   |
| E11 | 1     | PASPHEN/BI     |
| E12 | 1     | PASPHENE/BI    |

=> s e3

L1 6 PASPALININE/BI

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

5.40

5.61

FILE 'CAPLUS' ENTERED AT 19:15:53 ON 29 AUG 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 29 Aug 2007 VOL 147 ISS 10

FILE LAST UPDATED: 28 Aug 2007 (20070828/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s l1/prep

|    |                   |
|----|-------------------|
|    | 33 L1             |
|    | 4453515 PREP/RL   |
| L2 | 8 L1/PREP         |
|    | (L1 (L) .PREP/RL) |

=> s l2 and journal/dt

|    |                     |
|----|---------------------|
|    | 20063032 JOURNAL/DT |
| L3 | 7 L2 AND JOURNAL/DT |

=> d 1-7 ibib abs

L3 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:1199097 CAPLUS

DOCUMENT NUMBER: 147:8530

TITLE: Production of indole diterpenes by *Aspergillus*

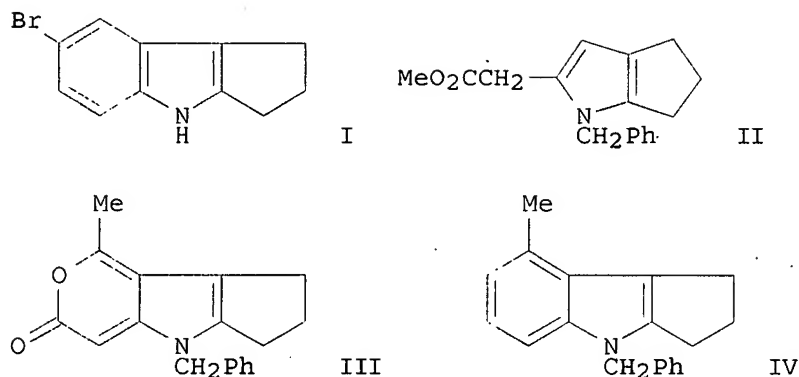
alliaceus  
AUTHOR(S): Junker, B.; Walker, A.; Cannors, N.; Seeley, A.;  
Masurekar, P.; Hesse, M.  
CORPORATE SOURCE: Merck Research Laboratories, Fermentation Development  
and Operations, Rahway, NJ, 07065, USA  
SOURCE: Biotechnology and Bioengineering (2006), 95(5),  
919-937  
CODEN: BIBIAU; ISSN: 0006-3592  
PUBLISHER: John Wiley & Sons, Inc.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Production of two related indole diterpenes (differing by a di-Me leucine side chain) by *Aspergillus alliaceus* was improved through several pilot scale ferms. Media were optimized through focus primarily on initial increases, as well as mid-cycle addns., of carbon and nitrogen sources. Fermentation conditions were improved by varying ventilation conditions using various combinations of air flowrate and back-pressure set points. Production improvements were quantified based on total indole diterpene concentration as well as the ratio of the major-to-minor byproduct components. Those changes with a pos. substantial impact primarily on total indole diterpene concentration included early cycle glycerol shots and enhanced ventilation conditions (high air flowrate, low back-pressure). Those changes with a significant impact primarily on the ratio included higher initial cerelose, soybean oil, monosodium glutamate, tryptophan, or ammonium sulfate concns., higher broth pH, and enhanced ventilation conditions. A few changes (higher initial glycerol and monosodium glutamate concns.) resulted in less notable and desirable titer or ratio changes when implemented individually, but they were adopted to more fully realize the impact of other improvements or to simplify processing. Overall, total indole diterpene titers were improved at the 600 L pilot scale from 125-175 mg/L with a ratio of about 2.1 to 200-260 mg/L with a ratio of about 3.3-4.5. Thus, the ability to optimize total indole diterpene titer and/or ratio readily exists for secondary metabolite production using *Aspergillus* cultures.

REFERENCE COUNT: 83 THERE ARE 83 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT .

L3 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:560774 CAPLUS  
DOCUMENT NUMBER: 123:56337  
TITLE: Cyclopenta[b]indoles. Part 2. Model studies towards  
the tremorgenic mycotoxins  
AUTHOR(S): Harrison, Carrie-Ann; Jackson, P. Mark; Moody,  
Christopher J.; Williams, Jonathan M. J.  
CORPORATE SOURCE: Dep. of Chemistry, Loughborough Univ. of Technology,  
Leicestershire, LE11 3TU, UK  
SOURCE: Journal of the Chemical Society, Perkin Transactions  
1: Organic and Bio-Organic Chemistry (1995), (9),  
1131-6  
CODEN: JCPRB4; ISSN: 0300-922X  
PUBLISHER: Royal Society of Chemistry  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 123:56337  
GI



AB The 7-bromocyclopenta[b]indole I has been converted into the hydroxybutenyl derivs. and a tetrahydrofuranylidene derivative in model studies towards the elaboration of paspalitrem and lolitrem type side chains. In a parallel approach, the cyclopentapyrrole II was converted into the fused  $\alpha$ -pyrone III which acted as a pyrrole-2,3-quinodimethane, and underwent Diels-Alder reaction to give, after loss of carbon dioxide, the cyclopentaindoles, e.g. IV.

L3 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1992:129335 CAPLUS  
 DOCUMENT NUMBER: 116:129335  
 TITLE: Total syntheses of (+)-paspalicine and (+)-paspalinine  
 AUTHOR(S): Sunazuka, T.; Smith, A. B., III; Leenay, T. L.; Wood, J. K.  
 CORPORATE SOURCE: Res. Cent. Biol. Funct., Kitasato Inst., Japan  
 SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1991), 33rd, 172-9  
 CODEN: TYKYDS  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Japanese

AB A symposium on the total synthesis of the title compds. in which a unified strategy in synthesis of (-)-paspaline is exploited.

L3 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1992:129296 CAPLUS  
 DOCUMENT NUMBER: 116:129296  
 TITLE: Indole diterpene synthetic studies. 8. The total synthesis of (+)-paspalicine and (+)-paspalinine  
 AUTHOR(S): Smith, Amos B., III; Kingery-Wood, Jill; Leenay, Tamara L.; Nolen, Ernest G.; Sunazuka, Toshiaki  
 CORPORATE SOURCE: Dep. Chem., Univ. Pennsylvania, Philadelphia, PA, 19104, USA  
 SOURCE: Journal of the American Chemical Society (1992), 114(4), 1438-49  
 CODEN: JACSAT; ISSN: 0002-7863  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 116:129296  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The development of a unified synthetic strategy for the indole diterpene tremorgens has led to the first total syntheses of (+)-paspalicine (I; R = H) and (+)-paspalinine (I; R = OH), in 22 and 23 steps, resp. The

cornerstone of the approach is the intermediacy of (-)-II this proposed common precursor to the simple indole diterpenes was previously generated in nine steps from (+)-Wieland-Miescher ketone (III) in an earlier synthesis of (-)-paspaline. Key transformations include installation of the indole unit via the Gassman protocol, alkylation of the thermodyn. anion of dimethylhydrazone IV with epoxide (-)-V, and RhCl<sub>3</sub>-promoted isomerization of the  $\beta,\gamma$ -unsatd. ketone in (+)-VI to afford I (R = H). I (R = OH) in turn was secured via SeO<sub>2</sub> oxidation of I (R = H), a particularly noteworthy result given the importance of the C(4b) hydroxyl group for tremorgenic activity. MM2 calcns. revealed that I embody the less stable relative configuration of the F- and G-ring bicyclic ketal moiety.

L3 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1991:207536 CAPLUS  
DOCUMENT NUMBER: 114:207536  
TITLE: Total syntheses of (+)-paspalicine and (+)-paspalinine  
AUTHOR(S): Smith, Amos B., III; Sunazuka, Toshiaki; Leenay, Tamara L.; Kingery-Wood, Jill  
CORPORATE SOURCE: Monell Chem. Senses Cent., Univ. Pennsylvania, Philadelphia, PA, 19104, USA  
SOURCE: Journal of the American Chemical Society (1990), 112(22), 8197-8  
CODEN: JACSAT; ISSN: 0002-7863  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 114:207536  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

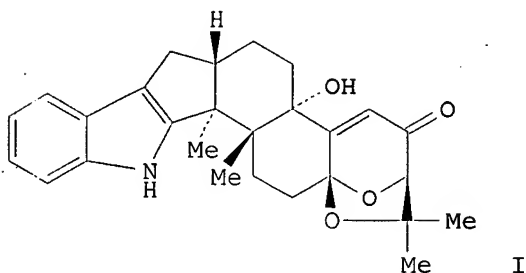
AB Total syntheses of the indole diterpenes (+)-paspalicine (I) (R = H) (II) and paspalanine I (R = OH) were achieved in 22 and 23 steps, resp., via a unified strategy applicable to the entire class of simple indole tremorgens. The intermediacy of tricyclic ketone III prepared in 9 steps from (+)-Wieland-Miescher ketone, served as the starting material for this approach. Central features of the scheme included installation of the indole unit via the Gassman protocol, construction of rings F and G by alkylation of the thermodyn. anion of the dimethylhydrazone of (+)-IV with epoxide (-)-V, and an RhCl<sub>3</sub>-promoted migration of the  $\beta,\gamma$ -olefinic bond in (+)-VI to afford II. (+)-Paspalinine in turn was secured via SeO<sub>2</sub> oxidation of II. The latter transformation is important given the requirement of a C(4b) tertiary hydroxyl group for tremorgenic activity.

L3 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1988:109279 CAPLUS  
DOCUMENT NUMBER: 108:109279  
TITLE: Novel indoloditerpenes, emindoles, and their related compounds from Emericella spp  
AUTHOR(S): Nozawa, Kohei; Nakajima, Seiichi; Kawai, Kenichi; Udagawa, Shunichi; Horie, Yoshikazu; Yamazaki, Mikio  
CORPORATE SOURCE: Fac. Pharm. Sci., Hoshi Univ., Japan  
SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1987), 29, 637-43  
CODEN: TYKYDS  
DOCUMENT TYPE: Journal  
LANGUAGE: Japanese  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB In the course of survey of paxilline (I) in *Emericella* spp., new-type indoloditerpenes, emindoles DA (II) and DB (III), and emindole SA (IV), were isolated from the mycelial extract of *E. desertorum* and *E. striata*, resp. The structure of II, III, and IV were determined on the basis of the spectroscopic and chemical data of their derivs. and x-ray crystallog. of emindole DA monoacetate. Three new compds. related to I, emindole SB, dehydroxypaxilline, and paxilline acetate, were also isolated along with I and paspaline from the mycelium of *E. striata*, and their structures were elucidated by the spectroscopic and chemical investigation. Two different types of indoloditerpenes, emindole SA and paxilline analogs (paspaline, emindole SB, dehydroxypaxilline, and paxilline acetate) were isolated from the same fungus, *E. striata*. Isolation of paspaline, emindole SB, dehydroxypaxilline and paxilline acetate from the same fungus may suggest the biogenesis of I.

L3 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1980:446901 CAPLUS  
DOCUMENT NUMBER: 93:46901  
TITLE: Paspalinine, a tremorgenic metabolite from *Claviceps paspali* Stevens et Hall  
AUTHOR(S): Gallagher, Rex T.; Finer, Janet; Clardy, Jon; Leutwiler, Albert; Weibel, Franz; Acklin, Werner; Arigoni, Duilio  
CORPORATE SOURCE: Dep. Chem., Cornell Univ., Ithaca, NY, 14853, USA  
SOURCE: Tetrahedron Letters (1980), 21(3), 235-8  
CODEN: TELEAY; ISSN: 0040-4039  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB The structure and absolute configuration of paspalinine (I) were determined by UV, IR, and NMR spectroscopy, and by x-ray crystallog.

=>

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

43.10

48.71

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-5.46

-5.46

FILE 'REGISTRY' ENTERED AT 19:40:21 ON 29 AUG 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 28 AUG 2007 HIGHEST RN 945714-55-6  
DICTIONARY FILE UPDATES: 28 AUG 2007 HIGHEST RN 945714-55-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

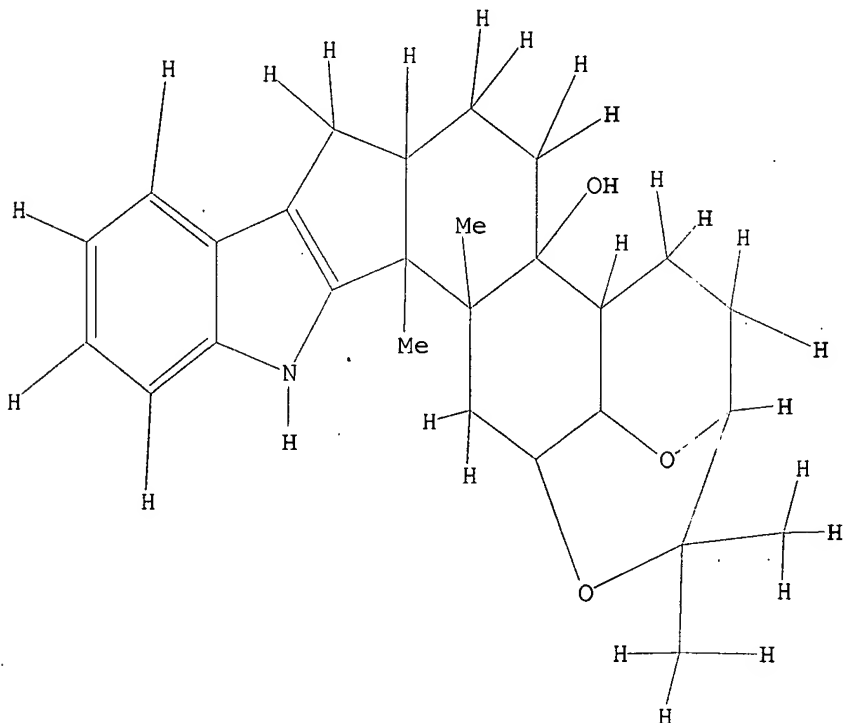
Uploading C:\Documents and Settings\pdickinson\My Documents\Paspalinine.str

L4 STRUCTURE UPLOADED

=> d l4

L4 HAS NO ANSWERS

L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l4

SAMPLE SEARCH INITIATED 19:40:51 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 84 TO ITERATE

100.0% PROCESSED 84 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 1131 TO 2229  
PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> s l4 full

FULL SEARCH INITIATED 19:40:55 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 1771 TO ITERATE

100.0% PROCESSED 1771 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L4

=> file caplus

|  |                  |               |
|--|------------------|---------------|
| COST IN U.S. DOLLARS                       | SINCE FILE ENTRY | TOTAL SESSION |
| FULL ESTIMATED COST                        | 172.10           | 220.81        |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE                        | 0.00             | -5.46         |

FILE 'CAPLUS' ENTERED AT 19:41:03 ON 29 AUG 2007  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 29 Aug 2007 VOL 147 ISS 10  
FILE LAST UPDATED: 28 Aug 2007 (20070828/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s l4

REGISTRY INITIATED  
Substance data SEARCH and crossover from CAS REGISTRY in progress...  
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 19:41:05 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 84 TO ITERATE

100.0% PROCESSED 84 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 1131 TO 2229  
PROJECTED ANSWERS: 0 TO 0

L7 0 SEA SSS SAM L4

L8 0 L7

=> file caplus

| COST IN U.S. DOLLARS                       | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| FULL ESTIMATED COST                        | 8.46             | 230.19        |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE                        | 0.00             | -5.46         |

FILE 'CAPLUS' ENTERED AT 19:51:50 ON 29 AUG 2007  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 29 Aug 2007 VOL 147 ISS 10  
FILE LAST UPDATED: 28 Aug 2007 (20070828/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> file reg

| COST IN U.S. DOLLARS                       | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| FULL ESTIMATED COST                        | 0.47             | 230.66        |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE                        | 0.00             | -5.46         |

FILE 'REGISTRY' ENTERED AT 19:51:52 ON 29 AUG 2007  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2007 American Chemical Society (ACS)



Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 AUG 2007 HIGHEST RN 945714-55-6  
DICTIONARY FILE UPDATES: 28 AUG 2007 HIGHEST RN 945714-55-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

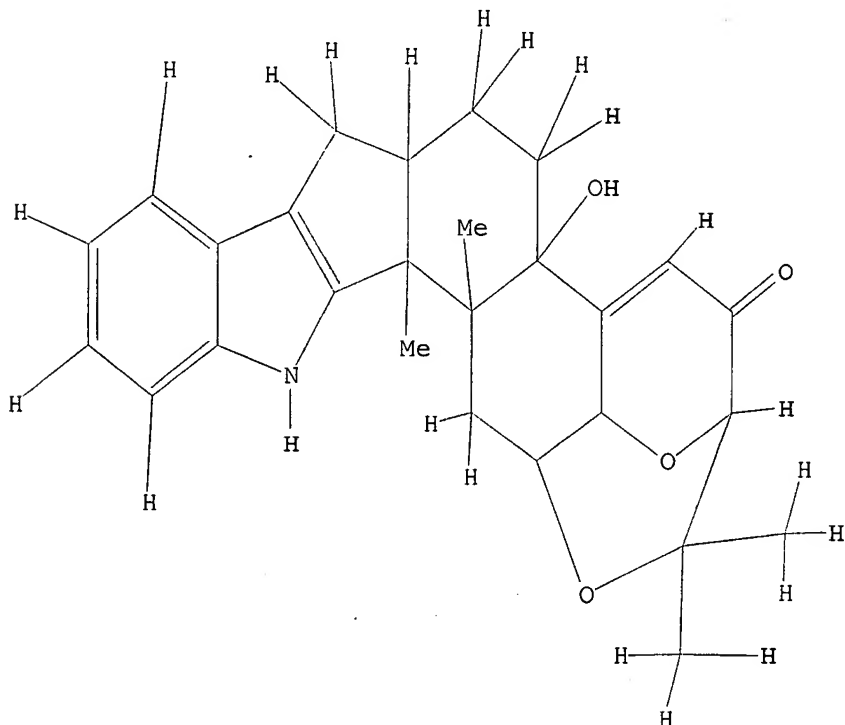
Uploading C:\Documents and Settings\pdickinson\My Documents\Literature Paspalinine.str

L9 STRUCTURE UPLOADED

=> d l9

L9 HAS NO ANSWERS

L9 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l19

L19 NOT FOUND

The L-number entered has not been defined in this session, or it has been deleted. To see the L-numbers currently defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>).

=> s l9

SAMPLE SEARCH INITIATED 19:52:33 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 84 TO ITERATE

100.0% PROCESSED 84 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 1131 TO 2229  
PROJECTED ANSWERS: 0 TO 0

L10 0 SEA SSS SAM L9

=> s l9 full

FULL SEARCH INITIATED 19:52:36 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 1771 TO ITERATE

100.0% PROCESSED 1771 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

L11 0 SEA SSS FUL L9

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> e paspalinine

|     |       |                |
|-----|-------|----------------|
| E1  | 2     | PASPALINIC/BI  |
| E2  | 1     | PASPALININ/BI  |
| E3  | 6 --> | PASPALININE/BI |
| E4  | 3     | PASPALITREM/BI |
| E5  | 4     | PASPALOIDES/BI |
| E6  | 35    | PASPALUM/BI    |
| E7  | 1     | PASPAT/BI      |
| E8  | 1     | PASPER/BI      |
| E9  | 5     | PASPER2/BI     |
| E10 | 1     | PASPERTIN/BI   |
| E11 | 1     | PASPHEN/BI     |
| E12 | 1     | PASPHENE/BI    |

=> s e3

L1 6 PASPALININE/BI

=> fil caplus

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST  | 5.40             | 6.45          |

FILE 'CAPLUS' ENTERED AT 17:27:52 ON 04 SEP 2007  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 4 Sep 2007 VOL 147 ISS 11  
FILE LAST UPDATED: 3 Sep 2007 (20070903/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s l1 and blocker

33 L1  
42236 BLOCKER  
37613 BLOCKERS  
65491 BLOCKER  
(BLOCKER OR BLOCKERS)  
L2 2 L1 AND BLOCKER

=> d l2

L2 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 2003:1006788 CAPLUS  
DN 140:53461  
TI Maxi-K potassium channel blockers for treatment of glaucoma and as ocular neuroprotective agents  
IN Goetz, Michael A.; Kaczorowski, Gregory J.; Monaghan, Richard L.; Strohl,

William R.; Tkacz, Jan S.  
 PA Merck & Co., Inc., USA  
 SO PCT Int. Appl., 50 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

|      | PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE     |
|------|---|------|----------|-----------------|----------|
| PI   | WO 2003105868   | A1   | 20031224 | WO 2003-US19013 | 20030613 |
|      | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,<br>CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,<br>GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,<br>LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH,<br>PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,<br>UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW<br>RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,<br>KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,<br>FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,<br>BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG |      |          |                 |          |
|      | CA 2488884  | A1   | 20031224 | CA 2003-2488884 | 20030613 |
|      | AU 2003245531   | A1   | 20031231 | AU 2003-245531  | 20030613 |
|      | EP 1515730  | A1   | 20050323 | EP 2003-739159  | 20030613 |
|      | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,<br>IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK  |      |          |                 |          |
|      | JP 2005538061   | T    | 20051215 | JP 2004-512770  | 20030613 |
|      | US 2005239787   | A1   | 20051027 | US 2004-511664  | 20041018 |
| PRAI | US 2002-389205P   | P    | 20020617 |                 |          |
|      | WO 2003-US19013   | W    | 20030613 |                 |          |

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d 2

L2 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1996:756504 CAPLUS  
 DN 126:26785  
 TI Effects of the K<sup>+</sup> channel blockers paspalitrem-C and paxilline  
 on mammalian smooth muscle  
 AU DeFarias, Fernando P.; Carvalho, Marcia F.; Lee, Seok H.; Kaczorowski,  
 Gregory J.; Suarez-Kurtz, Guilherme  
 CS Dep. Bioquim. Med., Univ. Fed. Rio de Janeiro, Rio de Janeiro,  
 RJ-21941-590, Brazil  
 SO European Journal of Pharmacology (1996), 314(1/2), 123-128  
 CODEN: EJPHAZ; ISSN: 0014-2999  
 PB Elsevier  
 DT Journal  
 LA English

=> s l1

L3 33 L1

=> s l1 and py<=2002

33 L1

22887930 PY<=2002

L4 28 L1 AND PY<=2002

=> d 1-28 ti

L4 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Toxigenic fungi in human environment

L4 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Effects of the K<sup>+</sup> channel blockers paspalitrem-C and paxilline on mammalian smooth muscle

L4 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Cyclopenta[b]indoles. Part 2. Model studies towards the tremorgenic mycotoxins

L4 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Antiinsectan alkaloids: shearinines A-C and a new paxilline derivative from the ascostromata of *Eupenicillium shearii*

L4 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI New paspalinine derivatives with antiinsectan activity from the sclerotia of *Aspergillus nomius*

L4 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Tremorgenic Indole Alkaloids Potently Inhibit Smooth Muscle High-Conductance Calcium-Activated Potassium Channels

L4 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Tremorgenic mycotoxins having indoloditerpene moiety

L4 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Indole antiinsectan *Aspergillus* metabolites.

L4 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Tremorgenic mycotoxins, paspalitrem A and C, from a tropical *Phomopsis*

L4 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Aflavarin and  $\beta$ -aflatrems: new anti-insectan metabolites from the sclerotia of *Aspergillus flavus*

L4 ANSWER 11 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Total syntheses of (+)-paspalicine and (+)-paspalinine

L4 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Indole diterpene synthetic studies. 8. The total synthesis of (+)-paspalicine and (+)-paspalinine

L4 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI The total synthesis of (+)-paspalicine and (+)-paspalinine

L4 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Isolation and determination of paspalitrem-type tremorgenic mycotoxins using liquid chromatography with diode-array detection

L4 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Total syntheses of (+)-paspalicine and (+)-paspalinine

L4 ANSWER 16 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Production of alfatrem and its related indoloditerpenes by microsclerotium-producing strains of *Aspergillus flavus*

L4 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Experimental constraints in the study of the biosynthesis of indole alkaloids in fungi

L4 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Studies of fungal products. Part XXVI. Isolation and structures of two new indoloditerpenes related to aflavinine from a microsclerotium-producing strain of *Aspergillus flavus*

L4 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

TI Indole diterpene synthetic studies. 5. Development of a unified synthetic strategy; a stereocontrolled, second-generation synthesis of (-)-paspaline

L4 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Carbon-13 NMR spectroscopy of indole derivatives

L4 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Novel indoloditerpenes, emindoles, and their related compounds from *Emericella* spp

L4 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Action of tremorgenic mycotoxins on GABAA receptor

L4 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Standardized high-performance liquid chromatography of 182 mycotoxins and other fungal metabolites based on alkylphenone retention indexes and UV-VIS spectra (diode array detection)

L4 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI High-performance liquid chromatographic determination of profiles of mycotoxins and other secondary metabolites

L4 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Paspalitrem C, a new metabolite from sclerotia of *Claviceps paspali*

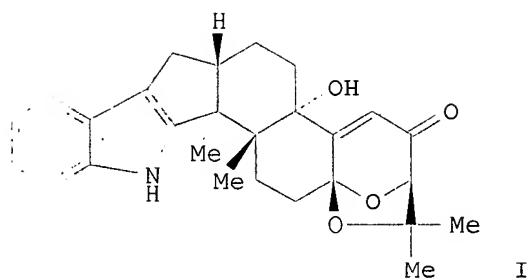
L4 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Indole metabolites from a strain of *Aspergillus flavus*

L4 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Paspalinine, a tremorgenic metabolite from *Claviceps paspali* Stevens et Hall

L4 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI *Paspalum* staggers: isolation and identification of tremorgenic metabolites from sclerotia of *Claviceps paspali*

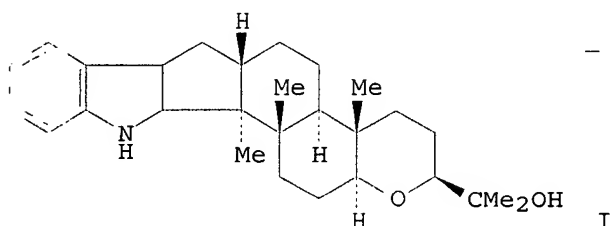
=> d 27, 25, 13, 12, 5, 1 ibib.abs

L4 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1980:446901 CAPLUS  
 DOCUMENT NUMBER: 93:46901  
 TITLE: Paspalinine, a tremorgenic metabolite from *Claviceps paspali* Stevens et Hall  
 AUTHOR(S): Gallagher, Rex T.; Finer, Janet; Clardy, Jon; Leutwiler, Albert; Weibel, Franz; Acklin, Werner; Arigoni, Duilio  
 CORPORATE SOURCE: Dep. Chem., Cornell Univ., Ithaca, NY, 14853, USA  
 SOURCE: Tetrahedron Letters (1980), 21(3), 235-8  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB The structure and absolute configuration of paspalinine (I) were determined by UV, IR, and NMR spectroscopy, and by x-ray crystallog.

L4 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1984:526410 CAPLUS  
 DOCUMENT NUMBER: 101:126410  
 TITLE: Paspalitrem C, a new metabolite from sclerotia of *Claviceps paspali*  
 AUTHOR(S): Dorner, Joe W.; Cole, Richard J.; Cox, Richard H.; Cunfer, Barry M.  
 CORPORATE SOURCE: Natl. Peanut Res. Lab., U.S. Dep. Agric., Dawson, GA, 31742, USA  
 SOURCE: Journal of Agricultural and Food Chemistry (1984), 32(5), 1069-71  
 CODEN: JAFCAU; ISSN: 0021-8561  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB A new metabolite was purified from  $\text{CHCl}_3$  exts. of *C. paspali* sclerotia by column chromatog. and preparative, centrifugally accelerated TLC. The chemical structure of the metabolite was determined by  $^1\text{H}$ - and  $^{13}\text{C}$ -NMR spectroscopy to be paspalitrem C (I). Paspalitrem C differed from the previously identified tremorgen, paspalitrem A, only by the position of attachment of the 3-methyl-2-butenyl unit to the indole ring.

L4 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1991:680346 CAPLUS  
 DOCUMENT NUMBER: 115:280346  
 TITLE: The total synthesis of (+)-paspalicine and (+)-paspalinine  
 AUTHOR(S): Klingery-Wood, Jill Elizabeth  
 CORPORATE SOURCE: Univ. Pennsylvania, Philadelphia, PA, USA  
 SOURCE: (1991) 266 pp. Avail.: Univ. Microfilms Int., Order No. DA9125690  
 From: Diss. Abstr. Int. B 1991, 52(3), 1438-9  
 DOCUMENT TYPE: Dissertation  
 LANGUAGE: English

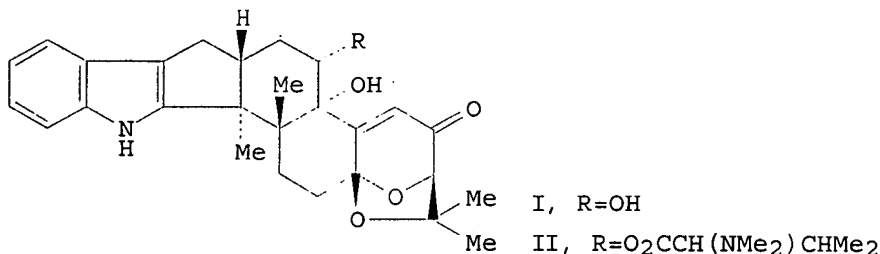
AB Unavailable

L4 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1992:129296 CAPLUS  
DOCUMENT NUMBER: 116:129296  
TITLE: Indole diterpene synthetic studies. 8. The total synthesis of (+)-paspalicine and (+)-paspalinine  
AUTHOR(S): Smith, Amos B., III; Kingery-Wood, Jill; Leenay, Tamara L.; Nolen, Ernest G.; Sunazuka, Toshiaki  
CORPORATE SOURCE: Dep. Chem., Univ. Pennsylvania, Philadelphia, PA, 19104, USA  
SOURCE: Journal of the American Chemical Society (1992), 114(4), 1438-49  
CODEN: JACSAT; ISSN: 0002-7863  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 116:129296  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The development of a unified synthetic strategy for the indole diterpene tremorgens has led to the first total syntheses of (+)-paspalicine (I; R = H) and (+)-paspalinine (I; R = OH), in 22 and 23 steps, resp. The cornerstone of the approach is the intermediacy of (-)-II this proposed common precursor to the simple indole diterpenes was previously generated in nine steps from (+)-Wieland-Miescher ketone (III) in an earlier synthesis of (-)-paspaline. Key transformations include installation of the indole unit via the Gassman protocol, alkylation of the thermodyn. anion of dimethylhydrazone IV with epoxide (-)-V, and RhCl<sub>3</sub>-promoted isomerization of the  $\beta,\gamma$ -unsatd. ketone in (+)-VI to afford I (R = H). I (R = OH) in turn was secured via SeO<sub>2</sub> oxidation of I (R = H), a particularly noteworthy result given the importance of the C(4b) hydroxyl group for tremorgenic activity. MM2 calcns. revealed that I embody the less stable relative configuration of the F- and G-ring bicyclic ketal moiety.

L4 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1994:293633 CAPLUS  
DOCUMENT NUMBER: 120:293633  
TITLE: New paspalinine derivatives with antiinsectan activity from the sclerotia of Aspergillus nomius  
AUTHOR(S): Staub, Gail M.; Gloer, Katherine B.; Gloer, James B.  
CORPORATE SOURCE: Dep. Chem., Univ. Iowa, Iowa City, IA, 52242, USA  
SOURCE: Tetrahedron Letters (1993), 34(16), 2569-72  
CODEN: TELEAY; ISSN: 0040-4039  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI





AB 14-Hydroxypaspalinine (I) and 14-(N,N-dimethyl-L-valyloxy)paspalinine (II) were isolated from the sclerotia of *Aspergillus nomius*, and identified by anal. of 2D NMR data. Both compds. caused 90% reduction in weight gain in assays against the corn earworm *Helicoverpa zea* at the 100 ppm (dry weight) dietary level. Paspalinine caused no effect at this concentration

L4 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:127616 CAPLUS  
DOCUMENT NUMBER: 136:305407  
TITLE: Toxigenic fungi in human environment  
AUTHOR(S): Krikstaponis, A.; Stakeniene, J.; Lugauskas, A.  
CORPORATE SOURCE: Institute of Botany, Vilnius, LT-2021, Lithuania  
SOURCE: Biologija (2001), (4), 10-12  
CODEN: BOLOE8; ISSN: 1392-0146  
PUBLISHER: Lietuvos Mokslu Akademijos Leidykla  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Fungal species compns. on vegetable-born food products and in the air and dust of dwellings were studied in 1996-2000. Seven food selling-storage places and 14 residences were investigated, 179 samples of 94 names of food products as well as 50 air and 118 dust samples were surveyed. Ability of 393 fungal isolates to produce secondary metabolites grown on Czapek - yeast extract and yeast extract - sucrose agar media was tested, 124 strains were regarded as active producers of secondary metabolities.

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT